On the origin dependence of multipole moments in electromagnetism.

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Abstract

The standard description of material media in electromagnetism is based on multipoles. It is well known that these moments depend on the point of reference chosen, except for the lowest order. It is shown that this "origin dependence" is not unphysical as has been claimed in the literature but forms only part of the effect of moving the point of reference. When also the complementary part is taken into account then different points of reference lead to different but equivalent descriptions of the same physical reality. This is shown at the microscopic as well as at the macroscopic level. A similar interpretation is valid regarding the "origin dependence" of the reflection coefficients for reflection on a semi infinite medium. We show that the "transformation theory" which has been proposed to remedy this situation (and which is thus not needed) is unphysical since the transformation considered does not leave the boundary conditions invariant.

1 Introduction

In classical electrodynamics[1] material media are modelled at the microscopic level as an ensemble of stable building blocks (atoms, ions, molecules, ...) with certain microscopic charge (η) and current ($\bar{j}$) densities. The microscopic fields

$(\overline{e},\overline{b})$ then obey the *microscopic* Maxwell equations:

$$\begin{aligned} \nabla\times\overline{e} &= -\frac{\partial\overline{b}}{\partial t} \qquad & \nabla\cdot\overline{b} &= 0 \\ \nabla\times\frac{\overline{b}}{\mu_0} &= \frac{\partial\varepsilon_0\overline{e}}{\partial t}+\overline{j} \qquad & \nabla\cdot\varepsilon_0\overline{e} &= \eta \end{aligned} \tag{1}$$

With a purely classical model the microscopic sources may be written as:

$$\eta = \sum_{k,l} q_{kl}\,\delta(\overline{r}-\overline{R}_{kl}) \qquad \overline{j} = \sum_{k,l} q_{kl}\dot{\overline{R}}_{kl}\,\delta(\overline{r}-\overline{R}_{kl}) \tag{2}$$

where the index k labels the building blocks and l the point charges (with position $\overline{R}_{kl}$ and velocity $\dot{\overline{R}}_{kl}$) within a building block. The *macroscopic* Maxwell equations then follow by a suitable averaging procedure. Due to the linearity these equations are similar to the ones in (1) with $(\overline{e},\overline{b})$ replaced by the macroscopic fields $(\overline{E},\overline{B})$ and with the microscopic sources replaced by their averages $(\langle\eta\rangle,\langle\overline{j}\rangle)$. The microscopic source densities (2) can be rearranged and expressed in terms of the (microscopic) electric and magnetic multipole moment densities. Usually only the 2 lowest order multipole moments are taking into account. After averaging, these lead to the usual macroscopic source densities:

$$\begin{aligned} \langle\eta\rangle &= \rho - \nabla\cdot\overline{P} \\ \langle\overline{j}\rangle &= \overline{J} + \frac{\partial\overline{P}}{\partial t} + \nabla\times\overline{M} \end{aligned} \tag{3}$$

where $(\rho,\overline{J})$ are the unbound charge and current densities and $\overline{P}$ and $\overline{M}$ the polarization and magnetization densities. In order to avoid the complexities associated with moving media, in what follows we will consider only non-moving media. Substituting (3) in the averaged (1) and defining $\overline{D}=\varepsilon_0\overline{E}+\overline{P}$ and $\overline{H}=\frac{\overline{B}}{\mu_0}-\overline{M}$ one finds the standard macroscopic Maxwell equations:

$$\begin{aligned} \nabla\times\overline{E} &= -\frac{\partial\overline{B}}{\partial t} \qquad & \nabla\cdot\overline{B} &= 0 \\ \nabla\times\overline{H} &= \frac{\partial\overline{D}}{\partial t}+\overline{J} \qquad & \nabla\cdot\overline{D} &= \rho \end{aligned} \tag{4}$$

If higher order multipole contributions are taken into account then additional terms show up in (3). By adapting the definition of $(\overline{D},\overline{H})$ accordingly equations (4) remain valid. However it should be noted that at a boundary between 2 media the jump conditions which follow from (4) have to be adapted in order to take into account these additional multipole contributions.

It is well known that the multipole moments are not unique and more precisely they depend on the choice of the reference point (e.g. the centre of mass) used for calculating the moments, except for the lowest order non vanishing moment. E.g. the total charge of an ion $q_k = \sum_l q_{kl}$ is independent of the reference point but the electric dipole moment is not, except if $q_k = 0$. For insulating materials the dipole terms are unique and since higher moments are usually not considered the non-uniqueness of the higher moments is often of no consequence.

In [2] [3] material media are treated up to the electric octopole and the magnetic quadrupole terms. The emphasis is on optical phenomena (in insulating media) and in particular Fresnel reflection coefficients are calculated for a semi-infinite medium taking into account these quadrupole and octopole effects. Therefore the authors are faced with the problem of the non-uniqueness of these higher order moments. As a result of lengthy calculations they find that in general those reflection coefficients also depend on the chosen reference point (it is called "origin dependent", but this should not be mistaken for the origin of the laboratory frame, but as a reference point within an atom.) These results are then discarded as being "unphysical" and using a "transformation theory" they adapt the "standard theory" so that "origin-independent" reflection coefficients are obtained. Although at first sight the reasoning may seem tempting no indication is given at what point exactly the "standard theory" became "unphysical". After some consideration we became convinced that there is actually no problem with the "standard theory" and that on the contrary the "origin dependence" as calculated in [2] has no physical meaning since only part of the effect of changing the position of the "origin" has been taken into account. In fact when choosing another reference point not only the higher order multipole moments do change but so does the position of these elementary sources. If both effects are taken into account then the microscopic charge density remains unchanged as expected. This is explained in more detail in section 2. In sections 3 and 4 the same idea is worked out in the macroscopic domain and in section 5 the effect on reflection coefficients is considered. It will become clear that there is no need for a "transformation theory". On the contrary, since the "standard theory" and the "transformation theory" give different results, at least one of them must be unphysical. In the last section 6 it will be shown that the "transformation theory" is unphysical since it does not leave the boundary conditions invariant.

2 Microscopic charge and current densities

In order to simplify the notation we consider only a single building block. Then up to quadrupole order the microscopic charge density is written as:

$$\eta = q\delta(\overline{r}-\overline{R}) - p_i\partial_i\delta(\overline{r}-\overline{R}) + q_{ij}\partial_{ij}\delta(\overline{r}-\overline{R}) + \cdots \tag{5}$$

where the electric multipole moments are defined as[4]:

$$\mu^{(n)} = \frac{1}{n!}\sum_l q_l \overline{r}_l^n \tag{6}$$

In (5) we use $\left(q, p_i, q_{ij}\right)$ as a shorthand notation for the 3 lowest order multipole moments, ∂_i for the derivative with respect to x_i, the cartesian components of $\overline{r}$, $\overline{R}$ for the position vector of the reference point and $\overline{r}_l$ for the position vector of charge l with respect to this reference point (thus $\overline{R}_l = \overline{R} + \overline{r}_l$, where compared with (2) the index k has been omitted). If we choose another reference point within the building block via $\overline{R} = \overline{R}' + \overline{d}$ and $\overline{r}_l = \overline{r}'_l - \overline{d}$ then in general different multipole moments are obtained:

$$p_i = \sum_l q_l x_{il} = \sum_l q_l (x'_{il} - d_i) = p'_i - qd_i \tag{7}$$

and similarly for the quadrupole moment:

$$q_{ij} = q'_{ij} - \frac{1}{2}(d_i p'_j + p'_i d_j) + \frac{1}{2} q d_i d_j \tag{8}$$

On the other hand these modified moments must now be placed in the new reference point. With a Taylor series we write:

$$\begin{aligned} \delta(\overline{r}-\overline{R}) &= \delta(\overline{r}-\overline{R}'-\overline{d}) \\ &= \delta(\overline{r}-\overline{R}') - d_i\partial_i\delta(\overline{r}-\overline{R}') + \frac{1}{2}d_i d_j \partial_{ij}\delta(\overline{r}-\overline{R}') + \cdots \end{aligned} \tag{9}$$

Inserting (7) (8) and (9) into (5) and retaining only terms up to quadrupole order one finds a similar expression but referred to the new reference point:

$$\eta = q\delta(\overline{r}-\overline{R}') - p'_i\partial_i\delta(\overline{r}-\overline{R}') + q'_{ij}\partial_{ij}\delta(\overline{r}-\overline{R}') + \cdots \tag{10}$$

Therefore the microscopic charge density (η) is as expected independent of the choice of reference point within the building block, although the multipole moments themselves do change according to (7) and (8). The interpretation is straightforward: suppose $q \neq 0$ then moving the reference point over $-\overline{d}$ changes

the dipole moment with $q\overline{d}$ but the monopole q must be moved with the reference point and this constitutes an additional dipole moment exactly cancelling the first change.

A similar conclusion can be drawn with respect to the microscopic current density. We define the magnetic multipole moments by:

$$\nu^{(n)} = \frac{n}{(n+1)!}\sum_l q_l \overline{r}_l^{n-1}(\overline{r}_l \times \dot{\overline{r}}_l) \tag{11}$$

with in particular for the magnetic dipole moment ($n = 1$):

$$m_i = \frac{1}{2}\sum_l q_l e_{ijk} x_{jl} \dot{x}_{kl} \tag{12}$$

where e_{ijk} is the Levi-Civita tensor. This dipole moment transforms according to:

$$m_i = m'_i - \frac{1}{2} e_{ijk} d_j \dot{p}'_k \tag{13}$$

Up to electric quadrupole and magnetic dipole order, the microscopic current density is then given by:

$$j_i = \dot{p}_i \delta(\overline{r} - \overline{R}) - \dot{q}_{ji}\partial_j \delta(\overline{r} - \overline{R}) + e_{ijk} m_k \partial_j \delta(\overline{r} - \overline{R}) \tag{14}$$

Substituting (7) (8) (13) and (9) into (14) again results in a similar expression for the microscopic current density with respect to the new reference point:

$$j_i = \dot{p}'_i \delta(\overline{r} - \overline{R}') - \dot{q}'_{ji}\partial_j \delta(\overline{r} - \overline{R}') + e_{ijk} m'_k \partial_j \delta(\overline{r} - \overline{R}') \tag{15}$$

We consider now as an example the reflection of a plane wave impinging on a semi infinite medium as was treated in [2]. In principle the problem could be solved at the microscopic level and this would result in definite values for the charge and current densities in each atom of the medium and thus for the global η and $\overline{j}$. We could then describe these resulting charge and current densities using multipole moments up to some chosen order and as shown this representation is independent of the choice of reference point, although the moments themselves are "origin dependent". This shows that already at the microscopic level the "origin dependence" of the multipole moments has no physical consequence supposed they are treated in a consequent way, meaning that the multipoles should be placed at their particular reference point.

3 Macroscopic charge and current densities

Since the macroscopic charge and current densities ($\langle\eta\rangle$, $\langle\overline{j}\rangle$) are obtained by averaging the microscopic densities, this conclusion must extend to the macroscopic level. The proper way of averaging is over an ensemble [5] with a probability density $f(\overline{R}_{kl},\dot{\overline{R}}_{kl};t)$ which depends on the positions of all charges and their velocities. Alternatively the probability can be expressed as a function of the atomic positions $\left(\overline{R}_k,\dot{\overline{R}}_k\right)$ and the internal coordinates $\left(\overline{r}_{kl},\dot{\overline{r}}_{kl}\right)$. Since the probability of finding the system in a particular configuration is independent of the choice of the atomic reference point it follows that:

$$f(\overline{R}_k,\dot{\overline{R}}_k,\overline{r}_{kl},\dot{\overline{r}}_{kl};t) = f'(\overline{R}'_k,\dot{\overline{R}}'_k,\overline{r}'_{kl},\dot{\overline{r}}'_{kl};t) \tag{16}$$

where we have already taken into account that the Jacobian of the transformation ($\overline{R}_k = \overline{R}'_k + \overline{d}$, $\overline{r}_{kl} = \overline{r}'_{kl} - \overline{d}$) equals unity. If we take the sum over all building blocks of the first contribution in (5) and take the average over this distribution function, we find the unbound charge density ρ in (3):

$$\rho = \langle\sum_k q_k \delta(\overline{r} - \overline{R}_k)\rangle = \sum_k q_k \int \delta(\overline{r} - \overline{R}_k) f_k(\overline{R}_k;t) d\overline{R}_k = \sum_k q_k f_k(\overline{r};t) \tag{17}$$

where $f_k(\overline{r};t)$ is the probability density for finding building block k at $\overline{r}$. Again for simplicity we consider now only the contribution of one particular kind of ions and (17) can then be written as:

$$\rho = q f_1(\overline{r};t) \tag{18}$$

where $f_1(\overline{r};t)$ is the probability density for finding 1 ion of this kind at $\overline{r}$. Note that (i) since we excluded moving media $\frac{\partial\rho}{\partial t} = 0$ and (ii) ρ should be supplemented with a contribution from the free electrons; but since these have no internal structure they are not relevant for our subject.

If we choose another reference point (shift of the origin) then in general another unbound charge density (due to the ions) is found:

$$\rho' = q f'_1(\overline{r};t) \tag{19}$$

Due to (16) the probability densities are related by $f_1(\overline{r};t) = f'_1((\overline{r} - \overline{d});t)$ and therefore $\rho(\overline{r}) = \rho'(\overline{r} - \overline{d})$. After developing we find:

$$\rho = \rho' - d_i \partial_i \rho' + \frac{1}{2} d_i d_j \partial_{ij} \rho' + \cdots \tag{20}$$

This result is completely similar with that found for the corresponding microscopic quantities where the δ-functions in the latter are here replaced by the

probability density function. The same reasoning can be followed for the higher order terms. For the polarization we find:

$$\overline{P} = \langle \sum_k \overline{p}_k \delta(\overline{r} - \overline{R}_k) \rangle = \int \overline{p}(\overline{r}_l) f_2(\overline{r}, \overline{r}_l; t) d\overline{r}_l \tag{21}$$

where the integration is over all internal coordinates and a similar expression holds for the shifted origin where the distribution functions are related by $f_2(\overline{r}, \overline{r}_l; t) = {f'}_2(\overline{r} - \overline{d}, \overline{r}'_l; t)$. Taking into account (7) and (19) we then find:

$$P_i(\overline{r}) = {P'}_i(\overline{r} - \overline{d}) - d_i \rho'(\overline{r} - \overline{d}) \tag{22}$$

where we have also taken into account that the integration of ${f'}_2$ over the internal coordinates yields ${f'}_1$ and where we have omitted the time dependence. After developing we find:

$$P_i = {P'}_i - d_i \rho' + d_i d_j \partial_j \rho' - d_j \partial_j {P'}_i + \cdots \tag{23}$$

For the quadrupole density we find in the same way:

$$Q_{ij}(\overline{r}) = {Q'}_{ij}(\overline{r} - \overline{d}) - \frac{1}{2}(d_i {P'}_j(\overline{r} - \overline{d}) + {P'}_i(\overline{r} - \overline{d}) d_j) + \frac{1}{2} d_i d_j \rho'(\overline{r} - \overline{d}) \tag{24}$$

and then up to quadrupole order:

$$Q_{ij} = {Q'}_{ij} - \frac{1}{2}(d_i {P'}_j + {P'}_i d_j) + \frac{1}{2} d_i d_j \rho' + \cdots \tag{25}$$

Although the individual multipole contributions do transform with a shift of the origin, according to (20) (23) (25) and so on, the total macroscopic charge density:

$$\langle \eta \rangle = \rho - \partial_i P_i + \partial_{ij} Q_{ij} + \cdots = \rho' - \partial_i {P'}_i + \partial_{ij} {Q'}_{ij} + \cdots \tag{26}$$

does not, as can readily be verified. A similar conclusion can be drawn with respect to the macroscopic current density $\langle \overline{j} \rangle$, which is given by:

$$\langle j_i \rangle = \partial_t P_i - \partial_t \partial_j Q_{ji} + e_{ijk} \partial_j M_k = \partial_t {P'}_i - \partial_t \partial_j {Q'}_{ji} + e_{ijk} \partial_j {M'}_k \tag{27}$$

where ∂_t is the partial derivative with respect to time and where the magnetization density transforms according to:

$$M_i(\overline{r}) = {M'}_i(\overline{r} - \overline{d}) - \frac{1}{2} e_{ijk} d_j \partial_t {P'}_k(\overline{r} - \overline{d}) \tag{28}$$

and then up to quadrupole order:

$$M_i = M'_i - \frac{1}{2} e_{ijk} d_j \partial_t P'_k \tag{29}$$

Since at the macroscopic level only $\langle \eta \rangle, \langle \overline{j} \rangle$ have physical meaning, whereas in general $\rho, P_i, Q_{ij}, M_i, \cdots$ do depend on the choice of reference point the latter must be considered as equivalent representations of the same physical macroscopic charge and current densities.

4 Polarizabilities

The constitutive equations of a medium express the response fields $P_i, Q_{ij}, M_i, \cdots$ as a function of the fields E_i, B_i. This dependence can be local in space and time or more in general the response fields can also depend on the values of the fields in nearby points and/or in the past. We will use the same linear expressions as in [2] (with slightly different notations) and we will consider only a non magnetic medium and again limit ourselves to terms of electric quadrupole/magnetic dipole order:

$$\begin{aligned} P_i &= P_i^{(0)} + \alpha_{ij} E_j + a_{ijk} \partial_j E_k + G_{ij} \partial_t B_j \\ Q_{ij} &= Q_{ij}^{(0)} + a_{kij} E_k \\ M_i &= M_i^{(0)} - G_{ji} \partial_t E_j \end{aligned} \tag{30}$$

The values of the multipole densities in the absence of any fields are indicated with a superscript (0). In [2] the origin dependence of the polarizabilities $\alpha_{ij}, a_{ijk}, G_{ij}, \cdots$ have been found based on a microscopic (and quantum mechanical) theory. Strictly speaking one should then consider first the local fields in (30) and then eliminate these so that only the macroscopic fields remain. We avoid this complication by considering (30) as pure macroscopic equations where the polarizabilities are phenomenological parameters. From the transformation properties of the response fields which have been found in the previous section we can deduce those of the polarizabilities.

Consider first the 2nd equation which we write in extenso as $Q_{ij}(\overline{r}) = Q_{ij}^{(0)}(\overline{r}) + a_{kij} E_k(\overline{r})$. A similar equation holds for the shifted reference point $Q'_{ij}(\overline{r}) = Q'^{(0)}_{ij}(\overline{r}) + a'_{kij} E_k(\overline{r})$. In view of (24) we combine these 2 into:

$$Q_{ij}(\overline{r} + \overline{d}) - Q'_{ij}(\overline{r}) = Q_{ij}^{(0)}(\overline{r} + \overline{d}) - Q'^{(0)}_{ij}(\overline{r}) + a_{kij} E_k(\overline{r} + \overline{d}) - a'_{kij} E_k(\overline{r}) \tag{31}$$

Using (24) twice this becomes:

$$-\frac{1}{2}d_i(P'_j(\overline{r})-P'^{(0)}_j(\overline{r}))-\frac{1}{2}(P'_i(\overline{r})-P'^{(0)}_i(\overline{r}))d_j=a_{kij}E_k(\overline{r}+\overline{d})-a'_{kij}E_k(\overline{r}) \tag{32}$$

On the left side we use the first equation of (30) only retaining terms up to quadrupole order (for the same reason the $\overline{d}$ on the right side can be dropped) and we then find:

$$a_{kij}=a'_{kij}-\frac{1}{2}(d_i\alpha'_{jk}+\alpha'_{ik}d_j) \tag{33}$$

In exactly the same way we find from the second equation in (30) and using (28):

$$G_{ij}=G'_{ij}+\frac{1}{2}e_{jkl}d_k\alpha'_{li} \tag{34}$$

Lastly from the first equation in (30) and using (22) we find at first:

$$\alpha_{ij}E_j(\overline{r}+\overline{d})+a_{ijk}\partial_jE_k(\overline{r}+\overline{d})+G_{ij}\partial_tB_j(\overline{r}+\overline{d})=\alpha'_{ij}E_j(\overline{r})+a'_{ijk}\partial_jE_k(\overline{r})+G'_{ij}\partial_tB_j(\overline{r}) \tag{35}$$

Equating the terms of dipole-order on both sides one finds:

$$\alpha_{ij}=\alpha'_{ij} \tag{36}$$

All terms of quadrupole order cancel each other if one uses (33), (34) and also takes into account Faraday's law $\partial_tB_j(\overline{r})=-e_{jkl}\partial_kE_l(\overline{r})$ and the symmetry of α_{ij}. The results (33) (34) and (36) are exactly the same as those found in [2], although they have been derived in a different way. Note that in transforming the polarizabilities we have taken into account that with the shift of the origin (for calculating the moments) one must also change the (position of the) driving field (see e.g. (35), where only the first $\left(\overline{r}+\overline{d}\right)$ expression is relevant due to our limitation to quadrupole order). It follows that if we use the origin dependencies of the polarizabilities as used in [2] and combine these with the proper shift of the field-point then the resulting macroscopic charge and current densities do not depend on the choice of origin as shown by (26) and (27).

5 Reflection coefficients

Turning now to the wave propagation in this medium it has been noted [2] that the (plane wave) modes are origin-independent. This was to be expected based on

the analysis given above. In order to determine the reflection coefficients for an air/medium interface we need the boundary or jump conditions at this interface, taking into account the quadrupole effects. Choosing the (x,y)-axes into the plane of the interface and with the z-axis pointing into the medium these can be written as:

$$\begin{aligned} \varepsilon_0 \Delta_s E_x &= \partial_x \mathscr{P}_z = -\partial_x Q_{zz} \\ \varepsilon_0 \Delta_s E_y &= \partial_y \mathscr{P}_z = -\partial_y Q_{zz} \end{aligned} \tag{37}$$

$$\varepsilon_0 \Delta_s E_z = \pi_s = -P_z + \partial_x Q_{zx} + \partial_y Q_{zy} + \partial_j Q_{jz} \tag{38}$$

$$\begin{aligned} \frac{\Delta_s B_x}{\mu_0} &= -K_y = -M_x + \partial_t Q_{zy} \\ \frac{\Delta_s B_y}{\mu_0} &= K_x = -M_y - \partial_t Q_{zx} \end{aligned} \tag{39}$$

$$\Delta_s B_z = 0 \tag{40}$$

where Δ_s stands for the field on the air side minus the field in the medium. π_s is the (bound) surface charge density, K_x, K_y are the components of the (bound) surface current density and $\mathscr{P}_x, \mathscr{P}_y, \mathscr{P}_z$ those of the surface polarization density. These equations are the same as those used in [2] except for (38) where the contribution $\partial_z Q_{zz}$ in the last term on the RHS is missing in [2] (and the conditions differ from those published previously [6]). The quadrupole contributions in (37)-(39) can be understood as follows: in the bulk of the medium the quadrupole density is equivalent with a polarization density $P_i^Q = -\partial_j Q_{ji}$. At the interface this density becomes singular and gives rise to a surface polarization density $\mathscr{P}_i = -Q_{zi}$. The normal component $\mathscr{P}_z = -Q_{zz}$ gives rise to a local voltage difference over the boundary and its variation along the boundary enters Faraday's law and explains (37). The in-plane components on the other hand give rise to a surface charge density $-\partial_x \mathscr{P}_x - \partial_y \mathscr{P}_y$, which explains the first 2 quadrupole contributions in (38), and a surface current density with components $\partial_t \mathscr{P}_x$ and $\partial_t \mathscr{P}_y$, which explain the contributions in (39). In the bulk the polarization $P_i^Q = -\partial_j Q_{ji}$ is equivalent with a charge density $-\partial_i P_i^Q = \partial_i \partial_j Q_{ji}$ and a current density $\partial_t P_i^Q = -\partial_t \partial_j Q_{ji}$. The former has a singularity at the surface leading to a surface charge density $\partial_j Q_{jz}$, which is the last contribution in (38). Note that without this term the normal component of the accompanying current density is not balanced at the surface.

Using Faraday's law on both sides of the interface it is easily seen that (37) implies (40). Similarly using instead Ampère's law one can also verify that (39) implies (38). Therefore we only need the equations (37) and (39) to find the reflection coefficients. In general the quadrupole contributions in these equations

will change if another reference point is chosen, as in the bulk of the material. However just as in the bulk this change will be balanced exactly by the displacement of the (lower order) dipole moment and therefore if calculated correctly no change in reflection coefficients should be found. However whereas in the bulk the latter effect is accounted for automatically (and yields an origin independent wave equation and origin independent modes) at the free surface it must be taken into account explicitly. It seems indeed logical that when moving the (atomic) reference point, and therefore all multipoles, over a distance $\overline{d}$, then one should at the macroscopic level, move the boundary surface over the same distance with the immediate conclusion that only d_z will be relevant. The effect of such a shift (alone) on the reflection coefficients is easily found to first order as:

$$(dR)_{\rm ss} = -2jk_z d_z R \tag{41}$$

where "ss" stands for "surface shift" and with k_z the normal wave vector component in free space (we use the time dependence $e^{j\omega t}$). If the reflection coefficients are origin independent then the change in the reflection coefficients due to the change of the quadrupole moments alone must exactly be opposite to the one in (41):

$$(dR)_{\rm qc} = 2jk_z d_z R \tag{42}$$

where "qc" stands for "quadrupole change" and this should be true irrespective of any symmetry properties of the medium. Proving this relation by direct analytical calculation turns out too complex so far in the most general case, this means for oblique incidence on an arbitrary medium[1]. However we could prove relation (42) if we relax one of these conditions: (i) perpendicular incidence on an arbitrary medium or (ii) oblique incidence on a medium with a 4-fold symmetry axis perpendicular to the surface. Further evidence for the general validity of (42) can be gathered directly from the relevant boundary conditions (37) and (39). Using (25) and (29) the changes in $\mathscr{P}_z, K_x, K_y$ due to the change of the quadrupole moment are given by[2]:

$$\begin{aligned} (d\mathscr{P}_z)_{\rm qc} &= d_z P_z \\ (dK_x)_{\rm qc} &= d_z \partial_t P_x \\ (dK_y)_{\rm qc} &= d_z \partial_t P_y \end{aligned} \tag{43}$$

Since the bulk current density has components $\partial_t P_x, \partial_t P_y$ along the free surface these variations are indeed as if the surface moved outwards over d_z whereas $d_z >$

[1] "arbitrary" means in this context "without any special symmetry properties".

[2] Note that due to our definition of $\overline{d}$ ($\overline{R} = \overline{R}' + \overline{d}$) the difference equals unaccented quantities minus accented quantities.

0 actually represents an inward movement of the surface, since the z-axis points into the medium. Finally we note that the lowest order term shown in (42) is imaginary since it corresponds with a pure phase shift. In [2] the variation of the modulus of R only was considered and therefore the relevant lowest order contribution to dR was missed. The variation of the modulus is indeed of a higher than quadrupole order and since calculations have been done up to quadrupole order only this is a meaningless result.

6 Transformations

In the frequency-domain the constitutive equations can generally be expressed as:

$$\begin{aligned} D_i &= \varepsilon_{ij} E_j + \gamma_{ij} B_j \\ H_i &= \beta_{ij} E_j + \nu_{ij} B_j \end{aligned} \tag{44}$$

where the material constants can be calculated from (30):

$$\begin{aligned} \varepsilon_{ij} &= \varepsilon_0 \delta_{ij} + \alpha_{ij} + jk_m(a_{jmi} - a_{imj}) \\ \gamma_{ij} = j\omega G_{ij} \qquad \beta_{ij} &= j\omega G_{ji} \qquad \nu_{ij} = \mu_0^{-1} \delta_{ij} \end{aligned} \tag{45}$$

Due to (33), (34) these material constants will usually be "origin dependent" and therefore at first sight also material dependent properties like e.g. reflection coefficients. As explained in the previous section the change of reference point should be accompanied by a shift of the free surface boundary and when both effects are taking into account the reflection coefficients are invariant. Raab and De Lange[2] [3] [7] did not take the latter effect into account but instead, in order to get rid of the "origin dependence" of the material constants in (45), they developed a "transformation theory", which essentially applies changes ΔG_{ij} and Δa_{ijk} to the polarizabilities in such a way that Maxwell's equations remain invariant. The new formulation is supposed to be equivalent with the original one, but since both formulations lead to different physical results (in casu different reflection coefficients) this cannot be true. This is due to the fact that no attention was given to the boundary conditions. In fact it is almost inescapable that different reflection coefficients (in casu origin independent ones) could only have been obtained using this procedure by changing the boundary conditions.

In order for the boundary conditions (37) and (39) to be invariant the RHS terms should not change by the transformation, since the fields $\overline{E}$ and $\overline{B}$ are unique, thus:

$$\Delta Q_{zz} = 0 \qquad \Delta K_x = 0 \qquad \Delta K_y = 0 \tag{46}$$

With (30) and since these conditions should hold for an arbitrary electric field it follows that:

$$\begin{aligned} \Delta a_{jzz} &= 0 \\ -\Delta G_{jy} + \Delta a_{jzx} &= 0 \\ \Delta G_{jx} + \Delta a_{jzy} &= 0 \end{aligned} \tag{47}$$

for any j. Since in addition boundary conditions should remain invariant along any possible boundary (not only the (x,y)-plane considered in this example) these conditions should also hold after cyclic permutation $x \to y \to z$. It then readily follows that $\Delta G_{ij} = 0$ and $\Delta a_{ijk} = 0$ meaning that no transformation leaves the boundary conditions invariant.

7 Conclusions

Changing the point of reference for calculating the multipole moments for the building blocks of a medium has two consequences. The moments themselves usually change with the reference point and the position in space of these elementary multipoles changes. If both effects are taken into account then the resulting charge and current densities are independent of the reference point. This has been shown at the microscopic and at the macroscopic level. The same interpretation can be applied to e.g. the reflection coefficients for a semi infinite medium: if with a change of origin the boundary of the medium is shifted accordingly, then the reflection coefficients are invariant. If the shift of the boundary is not taken into account then the reflection coefficient will show a variation corresponding with a pure phase shift. There is no need to remedy this "origin dependence" effect with a "transformation theory". In fact there is no transformation which leaves all possible boundary conditions invariant. We have performed all calculations including the multipoles of electric quadrupole/magnetic dipole order and for a non-magnetic and non-absorbing medium but we have no doubt that these results are still valid for more general materials.

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